

Finite Temperature Schrödinger Equation

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Abstract

We know Schrödinger equation describes the dynamics of quantum systems, which don't include temperature. In this paper, we propose finite temperature Schrödinger equation, which can describe the quantum systems in an arbitrary temperature. When the temperature $T = 0$, it become Schrödinger equation.

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1. Introduction

High-temperature and dense matter of elementary particles appears in several areas of physics. The first and most familiar example is the Universe at the early stages of its expansion. The Big Bang theory states that the Universe was hot and dense in the past [1,2], with a temperature ranging from a few eV up to the Planck scale. Another place, where matter exists in extreme conditions of high densities, can be created in the laboratory. Namely, in heavy-ion collisions extended dense fireballs of nuclear matter are created, with the energy density exceeding the QCD scale [3].

From a practical point of view, there is quite a wide area of applications of finite-temperature field theory to cosmology and laboratory experiments. The high-temperature phase transitions, typical for grand unified theories (GUTs), may be important for cosmological inflation and primordial density fluctuations. Topological defects can naturally arise at the phase transitions and influence the properties of the Universe we observe today. The first-order electroweak (EW) phase transition is a crucial element for electroweak baryogenesis; it may also play a role in the formation of the magnetic fields observed in the Universe. The QCD phase transition and properties of the quark-gluon plasma are essential for the understanding of the physics of heavy-ion collisions. The QCD phase transition in cosmology may influence the spectrum of the density fluctuations relevant to structure formation.

The construction of an effective action for quantum electrodynamics (QED) in the presence of various external conditions has been a challenge since the early days of the theory. The study of generalizations of the Heisenberg-Euler Lagrangian that include finite temperature effects has been initiated by Dittrich [4], who considered the case of a constant external magnetic field at finite temperature using the imaginary time formalism. An extension of this work to the case of arbitrary constant electromagnetic fields turned out to be qualitatively more substantial than naively expected. Employing the real-time formalism, this situation was investigated by Cox, Hellman and Yildiz [5], and Loewe and Rojas [6]. A more comprehensive study of the problem has been performed by Elmfors and Skagerstam [7], who corrected the preceding findings and additionally introduced a chemical potential. An attempt employing the imaginary-time formalism was made by

Ganguly, Kaw and Parikh [8] for the case of an external electric field. Recently, the finite-temperature effective action for electromagnetic fields was studied by Shovkovy [9] in the worldline approach, where finite temperature is also introduced via an imaginary-time formalism. In this paper, based on the first law of thermodynamics, we define the microscopic entropy of single particle and multi-particle, and give the finite temperature Schrödinger equations for the single particle and multi-particle, respectively.

2. The concept of microscopic and macroscopic entropy

In thermodynamics, the infinitesimal entropy change dS of a system is defined by

$$dS = \frac{\delta Q}{T}, \quad (1)$$

where δQ is a transfer of heat between the composite system and an external reservoir at the temperature T . In a finite change of state from i to j , the entropy change is $S_j - S_i$,

$$S_j - S_i = \int_i^j \frac{\delta Q}{T}, \quad (2)$$

The entropy of a system is a function of the thermodynamic coordinates whose change is equal to the integral of $\frac{\delta Q}{T}$ between the terminal states, integrated along any reversible path connecting the two states.

By integrating (1) around a reversible cycle, so that the initial and final entropies are the same. For a reversible cycle, we get

$$\oint \frac{\delta Q}{T} = 0. \quad (3)$$

In quantum statistics, the entropy S is defined by

$$S = -k_B \text{Tr}(\rho \ln \rho), \quad (4)$$

where $\rho = |\psi\rangle\langle\psi|$ is the density matrix, k_B is the Boltzmann constant.

In classical statistics, the entropy is defined by the Boltzmann

$$S = k_B \ln W = -k_B \ln \rho, \quad (5)$$

where W is the total number of the possible microscopic states, and $\rho = \frac{1}{W}$ is probability of every state.

From (5), we know that the macroscopic entropy is from the state distribution of a large number of particles. According to the viewpoint of macroscopic entropy, as the single particle hasn't state distribution, the single particle hasn't entropy.

In the viewpoint of quantum mechanics, a microscopic particle has wave-particle duality, and the wave nature is described by wave function. Obviously, the wave functions have the nature of distribution. So, a single particle has microscopic entropy, and we define its microscopic entropy S as

$$S = -k_w \ln |\psi(\vec{r}, t)|^2, \quad (6)$$

where k_w is a constant, which will be confirmed by experiment. The total microscopic entropy S is a functional of wave function ψ . It can be written as

$$S[\psi(\vec{r}, t)] = -k_w \ln |\psi(\vec{r}, t)|^2. \quad (7)$$

For the multi-particle system, the system total entropy is

$$S = -k_w \ln |\psi(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N, t)|^2. \quad (8)$$

where $\psi(\vec{r}_1, \vec{r}_2, \dots \vec{r}_N, t)$ is the total wave function of multi-particle system.

3. Finite temperature Schrödinger Equation

Based on the first law of thermodynamics, there is

$$dU = dW + dQ, \quad (9)$$

where dU is the infinitesimal change of system internal energy, dW is the infinitesimal work doing by surrounding, and dQ is the infinitesimal heat absorbed from surrounding. In this paper, we should study the quantum thermodynamics property of microscopic particles, i.e., finite temperature quantum theory of N-particle. When $dW = 0$, the (9) becomes

$$dU - dQ = 0. \quad (10)$$

For the point particle system of N-particle, the internal energy U is

$$U = \sum_{i=1}^N (T_i + V_i) + \sum_{i<j}^N V_{ij}, \quad (11)$$

where T_i and V_i are the i -th particle's kinetic energy and potential energy, and V_{ij} is the interaction energy of i -th and j -th particle, the internal energy infinitesimal change is

$$dU = d\left(\sum_{i=1}^N (T_i + V_i) + \sum_{i<j}^N V_{ij}\right), \quad (12)$$

since

$$dQ = \sum_{i=1}^N dQ_i = \sum_{i=1}^N T dS_i = d\left(\sum_{i=1}^N T S_i\right), \quad (13)$$

where dQ_i is the i -th particle absorbed heat, dS_i is the i -th entropy change. T is the system temperature.

By substituting (12), (13) into (10), we have

$$d\left(\sum_{i=1}^N (T_i + V_i) + \sum_{i<j}^N V_{ij} - T \sum_{i=1}^N S_i\right) = 0. \quad (14)$$

i.e.,

$$\sum_{i=1}^N (T_i + V_i) + \sum_{i<j}^N V_{ij} - TS = E, \quad (15)$$

where $S = \sum_{i=1}^N S_i$ is system total entropy, E is a constant, which can be defined as the total energy of system.

By canonical quantization

$$E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad T_i = -\frac{\hbar^2}{2m_i} \nabla_i^2, \quad (16)$$

and

$$S = -k_w \ln |\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t)|^2. \quad (17)$$

The (15) becomes quantum wave equation

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t) &= \left[\sum_{i=1}^N \left(-\frac{\hbar^2}{2m_i} \nabla_i^2 + V_i \right) + \sum_{i<j}^N V_{ij} \right. \\ &\quad \left. + k_w T \ln |\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t)|^2 \right] \psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t). \end{aligned} \quad (18)$$

The (18) is finite temperature Schrödinger equation of multi-particle. When $T = 0$, the (18) becomes Schrodinger equation of multi-particle system.

The partial differential (18) can be solved by the method of separation of variable. By writing

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N, t) = \psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) g(t), \quad (19)$$

submitting (19) into (18), we have

$$i\hbar \frac{dg(t)}{dt} - k_w T \ln g^2(t) \cdot g(t) = E g(t), \quad (20)$$

and

$$\begin{aligned} & \sum_{i=1}^N \left(-\frac{\hbar^2}{2m_i} \nabla^2 \psi(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N) + V(r_1, r_2 \cdots r_N) \right) \psi(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N) \\ & + \sum_{i < j}^N V_{ij} \psi(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N) + k_w T (\ln |\psi(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N)|^2) \psi(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N) \\ & = E \psi(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N). \end{aligned} \quad (21)$$

Equation (21) is time-independent finite temperature Schrödinger equation of multi-particle system.

For the single particle, the (15) becomes

$$\frac{p^2}{2m} + V - TS = E, \quad (22)$$

where $\frac{p^2}{2m}$, V and E are the single particle kinetic energy, potential energy and total energy, S is the single particle total microscopic entropy and T is the single particle's surrounding temperature. For a classical particle, its entropy is zero, and its total energy $E = \frac{p^2}{2m} + V$, i.e., its total energy is mechanical energy. For a microscopic particle, due to the wave nature, it has microscopic entropy. The microscopic particle total energy E is the sum of its mechanical energy $\frac{p^2}{2m} + V$ and $-TS$. We define $-TS$ as heat potential energy.

By canonical quantization

$$E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad T = -\frac{\hbar^2}{2m} \nabla^2, \quad (23)$$

and

$$S = -k_w \ln |\psi(\vec{r}, t)|^2, \quad (24)$$

the (22) becomes quantum wave equation

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}, t) + V \psi(\vec{r}, t) + k_w T (\ln |\psi(\vec{r}, t)|^2) \psi(\vec{r}, t). \quad (25)$$

The (25) is the finite temperature Schrodinger equation of single-particle. When $T = 0$, it becomes the single particle Schrodinger equation.

The partial differential (25) can be solved by the method of separation of variable. By writing

$$\psi(\vec{r}, t) = \psi(\vec{r})g(t), \quad (26)$$

submitting (26) into (25), we have

$$i\hbar \frac{dg(t)}{dt} - k_w T \ln g^2(t) \cdot g(t) = Eg(t), \quad (27)$$

and

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(r)\psi(\vec{r}) + k_w T (\ln |\psi(\vec{r})|^2) \psi(\vec{r}) = E\psi(\vec{r}). \quad (28)$$

Equation (28) is time-independent finite temperature Schrödinger equation of single-particle.

4. Conclusion

In this paper, we define microscopic entropy of single particle and multi-particle, and give the finite temperature Schrödinger equation of a single and multi-particle. With these equations, we can study quantum systems in an arbitrary temperature, such as superconductivity mechanism, Bose-Einstein condensates and so on.

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